Finite Element Model Characterization Of Nano-Composite Thermal And Environmental Barrier Coatings

Thermal and environmental barrier coatings have been applied for protecting Si based ceramic matrix composite components from high temperature environment in advanced gas turbine engines. It has been found that the delamination and lifetime of T/EBC systems generally depend on the initiation and propagation of surface cracks induced by the axial mechanical load in addition to severe thermal loads. In order to prevent T/EBC systems from surface cracking and subsequent delamination due to mechanical and thermal stresses, T/EBC systems reinforced with nano-composite architectures have showed promise to improve mechanical properties and provide a potential crack shielding mechanism such as crack bridging. In this study, a finite element model (FEM) was established to understand the potential beneficial effects of nano-compsoites systems such as SiC nanotube-reinforced oxide T/EBC systems.
Finite Element Model Characterization of Nano-Composite Thermal and Environmental Barrier Coatings

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The 35th International Conference on Advanced Ceramics and Composites
Daytona Beach, FL
January 23-28, 2011
Introduction

- Environmental barrier coating (EBC) systems are used for protecting Si-based ceramic hot section components.
- Nanotube composites, having extremely high stiffness and strength and functional properties, are currently being considered for EBC to improve the coating performance.
- In particular, SiC nanotubes (SiCNTs) are being incorporated into EBC bond coats to increase their strength and toughness.
Advantages of Nanotube Reinforcements

Nanotubes as compared to other micro scale reinforcements:

- Can achieve much higher volume fraction
- More crack arresters due to more interfaces
- Exhibit more homogenized material response
- Less stress concentration (Gradual stress distribution)

<table>
<thead>
<tr>
<th></th>
<th>Fiber</th>
<th>Wisker</th>
<th>Nanotube</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vf=20%</td>
<td>20 µm</td>
<td>1~5 µm</td>
<td>0.005~0.1 µm</td>
</tr>
<tr>
<td>r =</td>
<td>25 µm</td>
<td>1.3~6.5 µm</td>
<td>0.0065~0.130 µm</td>
</tr>
<tr>
<td>Spacing</td>
<td>2~3</td>
<td>8~50</td>
<td>800~4000</td>
</tr>
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<td>#</td>
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Improvement of toughness with SiCNT

HfO$_2$-SiCNT nano-composites, tested at 1450°C ($\Delta T=1000^\circ$C), with Random orientation SiCNT, Wavy, 5 μm long:

- HfO$_2$ + 0% SiCNT:
- HfO$_2$ + 20% SiCNT:
- HfO$_2$ + 40% SiCNT

➢ Higher volume fraction showed improved toughness/strength.
Outline

To understand mechanical improvement in toughness/strength

• Multiscale modeling approach for nano-composite property determination:
  o HfO$_2$ + SiCNT nano-composite model system

• FEA to determine micro (nano) scale properties

• Homogenization technique – Micromechanics Analysis Code (MAC/GMC)

• Results and discussions on effect of SiCNT architectures

• Summary
Approach to Determine Global Scale Mechanical Properties

\[ K = \sigma (\pi a)^{1/2}, \text{ where } \sigma = f(E, \Delta T, \ldots) \]

- Increasing stiffness \( E \) will improve toughness \( K \) for a given material system
- Multi-scale modeling approach is used to determine bulk composite stiffness

**Micro Scale**
- Fiber/Inclusion
- Interphase
- Matrix

**Meso Scale**
- Tow
- Ply
- Woven/Braided RUC
- Laminate

**Global Scale**
- Structure

**Steps**
1. **Atomistic Scale**
   - \( V_f \)
   - Length
   - Waviness
   - Orientation

2. **FEA**
3. **MAC/GMC**
   - Various Micro/Meso scale RVEs
   - Global scale Mechanical properties
FEA Simulation (Micro scale properties)

- Assuming perfect bond and equally distributed
- SiCNT: $E_{NT} = 600 \text{GPa}, \nu = 0.3$
- HfO$_2$ Matrix: $E_M = 100 \text{GPa}, \nu = 0.3$
- SiCNT radius: $r = 0.05 \, \mu\text{m (50 nm)}$
- SiCNT length: $L = 0.5, 1, 5, 10, 50 \, \mu\text{m}$
  \( r/L = 10, 20, 100, 200, 1000 \)
- Waviness: $\lambda = a/b = 0.0, 0.1, 0.2$
- Orientation: $\theta = 0, 30, 45, 60, 90^\circ$
- Volume fraction: $V_f = 0\sim 60 \%$

FEA model:
- Element Type: Hex20 and Wedge15
- # of Nodes: 3000 ~ 90000
- # of Elements: 400 ~ 15000
Micro Scale Properties: $V_f$ and Length effect

FEA simulation
Straight SiCNT:
Radius: $r = 0.05 \, \mu m$
Length: $L = 0.5 \, \mu m$

Loading direction

Transposed direction

Volume fraction, %
Micro Scale Properties: Effect of Waviness

FEA simulation

$V_f = 20\%$

Loading direction

$\lambda = 0.1$
$\lambda = 0$
$\lambda = 0.2$

Transposed direction

$\lambda = 0.2$
$\lambda = 0.1$
$\lambda = 0$

Length of SiCNT, $\mu$m

$E/E_M$

$3.0$

$2.8$

$2.6$

$2.4$

$2.2$

$2.0$

$1.8$

$1.6$

$1.4$

$1.2$
Micro Scale Properties: Summary (FEA simulation)

- $V_f = 20\%$
  - SiCNT
  - $L = 5 \mu m$

- $V_f = 40\%$
  - SiCNT
  - $L = 5 \mu m$
Homogenization (Micro to Macro by MAC/GMC)

- $1^{st}$ order Taylor series of displacement field
- Satisfy continuity of displacements & tractions between subcells
- Impose periodicity conditions on displacements and tractions at the unit cell boundaries

**Double Periodicity**

$\vec{\sigma} = B^* (\vec{\varepsilon} - \vec{\varepsilon}^I + \vec{\varepsilon}^T)$

\[
B^* = \frac{1}{dh} \sum_{a=1}^{N_a} \sum_{p=1}^{N_p} \sum_{l=1}^{N_l} d_a h_p l C^{(apfr)} A^{(apfr)}
\]

\[
\vec{\varepsilon}^I = \frac{-B^{-1}}{dh} \sum_{a=1}^{N_a} \sum_{p=1}^{N_p} \sum_{l=1}^{N_l} d_a h_p l C^{(apfr)} (D^{(apfr)} \vec{\varepsilon}_S^I - \vec{\varepsilon}^{I(apfr)})
\]

\[
\vec{\varepsilon}^T = \frac{-B^{-1}}{dh} \sum_{a=1}^{N_a} \sum_{p=1}^{N_p} \sum_{l=1}^{N_l} d_a h_p l C^{(apfr)} (D^{(apfr)} \vec{\varepsilon}_S^T - \vec{\varepsilon}^{T(apfr)})
\]

**Macro-level Constitutive Equations**

Provides effective constitutive equation for composite material

**Micro-level Field Equations (subcell)**

Provides access to local stresses and strains in fiber and matrix

Homogenization (Micro to Macro by MAC/GMC)

Double Periodicity

Triple Periodicity

- Straight SiCNT: Radius: \( r = 0.05 \mu m \)
- Length:
  - \( L = 0.5, 1.0, 5, 10, 50 \mu m \)

- MAC/GMC

Graph showing the relationship between E/E_M and volume fraction, %.
Macro Scale Properties for SiCNT Composites

Strain, $\varepsilon$ vs. Stress Ratio, $\sigma/\sigma_M$

- $L = 5 \, \mu m$
  - $V_I = 40\%$ SiCNT: $2.02$
  - $V_I = 20\%$ SiCNT: $1.67$

- $L = 50 \, \mu m$
  - $V_I = 40\%$ SiCNT: $2.07$
  - $V_I = 20\%$ SiCNT: $1.68$

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Improvement of toughness with SiCNT

HfO$_2$-SiCNT nano-composites, tested at 1450°C ($\Delta T=1000°C$), with Random orientation SiCNT, Wavy, 5 μm long:

\[ K = \sigma (\pi a)^{1/2}, \text{ where } \sigma = f (E, \Delta T, \ldots) \]

- **HfO$_2$ + 0% SiCNT:**
  - $E = E_m = 100$ GPa

- **HfO$_2$ + 20% SiCNT:**
  - $E = 1.67\sim1.68 \ E_m$
  - Toughness improvement: less than +67\sim68 \% 

- **HfO$_2$ + 40% SiCNT:**
  - $E = 2.02\sim2.07 \ E_m$
  - Toughness improvement: more than +102\sim107 \%
Summary

- Based on micromechanics modeling, relative improvement in toughness was investigated.
- $V_f$ of 20~40% showed optimum improvement in material properties.
- Waviness tends to improve transverse stiffness.
- $r/L$ (NT radius to length) ratio > 100 showed no improvement in stiffness.
- Totally random orientation with wavy and straight NT provided isotropic material behavior.
- Based on preliminary experiments, in order to prevent from surface cracking, 40% $V_f$ of SiCNT (+102% toughness improvement) is needed and 20% $V_f$ (+67% toughness improvement) was not sufficient.
Future Work

• Conduct classical fracture test (3pt bend specimen) and indentation test to measure fracture toughness
• Determine SiCNT strength and interfacial bonding strength from Molecular dynamics (MD) simulation

Acknowledgement

The work was supported by NASA Fundamental Aeronautics Program (FAP) Supersonics Project.